LigPrep Command Options

The syntax of the `ligprep` command is as follows.

`$SCHRODINGER/ligprep` [*options*|*meta-options*] {`-imae`|`-isd`|`-ismi`} *infile* {`-omae`|`-osd`} *outfile*

The options are listed in Table 1, grouped by stage. The meta-options are listed in Table 2, and the action of the meta-options is explained in Table 3. The `ligprep` command also supports the standard Job Control options, which are described in Section 2.3 of the *Job Control Guide*, and some other job options, which are listed in Table 4. Options for `para_ligprep` are listed in Table 5; `para_ligprep` passes any other options on to the `ligprep` command. `para_ligprep` is used to distribute LigPrep jobs over multiple processors, and has the same syntax as `ligprep`.

Table 1. Options for the `ligprep` *command*

Option	Definition
General	
`-a`	Append structures to the output file. Default is to overwrite the output file if it already exists.
`-inp` *filename*	Use input file to obtain values for options. Values given on the command line supersede values given in the input file.
`-kp` | `-keep_props`	Transmit properties from input to output at each stage, and retain properties in the output structure file. The `ionizer` and `bmin` delete properties by default.
`-ma` *number*	Skip over structures containing more than this number of atoms in some steps. Default: 150.
`-n` *structs*	Specify a comma-delimited series of colon-separated ranges and single values to convert. For example: `1:10,14` Structures 1 through 10, and 14 `2:` Structures 2 through end of file `:5,13:18` Structures 1 through 5, and 13 through 18 Default: `1:` (convert all structures)
`-nc`	Do not remove intermediate files. Default is to remove intermediate files.
`-np`	Remove files containing problematic structures. Default is to keep problematic structure files.

`-R {b|c|d|e|f|h|i|n|p|r|s|t}`	Run only the stage of ligand preparation specified by the letter code:
	`b` `bmin` minimization — `i` `ionizer`
	`c` `sdconvert` — `n` `neutralizer`
	`d` `desalter` — `p` `premin`
	`e` `epik` — `r` `ring_conf`
	`f` filter (`ligfilter`) — `s` `stereoizer`
	`h` `applyhtreat` — `t` `tautomerizer`

`-sif_docs`	Display documentation for the simplified input file, and exit.
`-verb`	Report on the progress of the ligand preparation.

`-W` *string*	Options for various stages of ligand preparation. *string* consists of comma-separated designators. The first designator specifies the program that options are to be passed to and must be one of:
	`ci` `sdconvert` on input structures
	`co` `sdconvert` on output structures
	`e` `epik`
	`f` filter (`ligfilter` or `ligparse`)
	`i` `ionizer`
	`qp` `qikprop`
	`r` `ring_conf`
	`s` `stereoizer`

Table 1. Options for the `ligprep` *command (Continued)*

Option	Definition
	The remaining designators are passed to the program in the order specified with the commas removed. For example: `r,-l,1,-n,16` passes the arguments `-l 1 -n 16` to `ring_conf`. Multiple `-W` options are permitted, but only the last one pertaining to a particular program is used. For `ring_conf` and `stereoizer`, these options are used in addition to the default options and override redundant specifications. When `ligparse` is in use, it is passed the following arguments by default: `-any -j 5` (filter by rejecting structures if any criteria listed in the filter file are matched). If the `-W` option is used to pass arguments to `ligparse`, the default set of arguments is not used by `ligparse`.
Desalting	
`-nd`	Do not use the `desalter`. Default is to use the `desalter`.
Ionization	
`-emb`	Use the Epik metal binding option for ionization and tautomerization of ligands bound to protein metals. An alternative form of this option is `-epik_metal_binding`.
`-epik`	Use Epik for the ionization and tautomerization stages.
`-es` *filename*	Use the specified nonstandard Epik pK_a file.
`-i` *number*	Ionization treatment `0` Do not neutralize or ionize. `1` Neutralize only. `2` Neutralize and ionize. Default: 1. Ionization is performed by default with the `ionizer`. If `-epik` is used, this option only controls neutralization.
`-is` *filename*	Use non-standard `ionizer` specification file, named *filename*.
`-mbs` *filename*	Use the specified nonstandard Epik metal binding file.
`-mg` *number*	Instruct `ionizer` to skip structures that have more than this number of ionizable groups. Default: 10
Tautomerization	
`-emb`	Use Epik metal binding option for ionization and tautomerization of ligands bound to protein metals. An alternative form of this option is `-epik_metal_binding`.
`-epik`	Use Epik for the ionization and tautomerization stages.
`-mbs` *filename*	Use the specified nonstandard Epik metal binding file.
`-nt`	Do not generate tautomers. Default is to generate tautomers.
`-t` *number*	Generate up to *number* tautomers per input structure. Default: 8
`-ts` *filename*	Specify a custom tautomer database.
`-tp` *number*	Set the minimum tautomerization probability to *number*, where 0 < *number* < 1.0. Structures with net tautomerization probabilities lower than this value are not retained. Default: 0.01
Stereoisomers	
`-ac`	Do not respect existing chirality properties or use chiralities from the input geometry. Generate stereoisomers for all chiral centers up to the number permitted (specified using the `-s` option).
`-g`	Respect chiralities from input geometry when generating stereoisomers. For chiral centers whose chirality cannot be determined from the input geometry, stereoisomers will be generated.
`-ns`	Do not generate stereoisomers. Chiral properties in the input file are still enforced. Default is to generate stereoisomers.
`-s` *number*	Generate up to *number* stereoisomers per input structure. Default: 32

Table 1. Options for the `ligprep` *command (Continued)*

Option	Definition
Ring conformations	
`-l` *number*	Control how `ring_conf` handles atoms that are not in flexible rings. `1` Use input geometries. `2` Use idealized geometries even for rigid rings. `3` Use idealized geometries for non-ring portions and input geometries for rigid rings. Default: 3
`-r` *number*	Generate up to *number* ring conformations per input structure. Default: 1
`-re` *number*	Generate ring conformations with energies lower than *number* (kJ/mol) relative to the lowest energy conformer. This number sets the maximum number of ring conformers to 8 unless a different number is provided using the `-r` option.
Filtering	
`-f` *filename*	Filter structures using filtering criteria from *filename*. Default: do not filter.
`-fc` *filename*	Use custom composite descriptors for `ligparse` from *filename*. Only valid when used with `-f` and `-use_ligparse`. Default: use composite descriptors from `composite.types` file in the installation.
`-fs` *filename*	Use custom SMARTS patterns (descriptors) for `ligparse` from *filename*. Only valid when used with `-f` and `-use_ligparse`. Default: use composite descriptors from `str_keys.types` file in the installation.
`-lab`	Add an internal tracking label that can be used for filtering.
`-lab_filter` *options*	Filter the output based on the tracking labels introduced with `-lab`, which is turned on by this option. The filtering process is controlled by the options. Only one option is supported: `ionizer:`*n*—select at most *n* output structures for each ionizer input structure such that the formal charge on each ionizable group is minimized.
`-lp`	Include calculated `ligfilter` properties in the output structure file. Not valid with `-use_ligparse`, which includes properties by default.
`-use_ligparse`	Use `ligparse` for filtering. Default: use `ligfilter`.
Final optimization	
`-bff` *number*	Instruct `bmin` to use the force field specified. Only 10 (MMFFs), 11 (OPLS_2001), and 14 (OPLS_2005, default) are supported.
`-bvac`	Perform `bmin` minimization in a vacuum. By default `bmin` minimizations are carried out using a distance-dependent dielectric.
`-br`	Instruct `bmin` to retain structures with incorrect chiralities.
`-bns`	Instruct `bmin` to perform minimizations only. By default, `bmin` performs short conformational searches on distorted structures.
`-btc` *number*	Torsional constraints to use in `bmin`. `-1` Do not use torsional constraints. `0`, `1` Torsional constraints for C=C, carboxylic acids, esters and amides. `2` Torsional constraints for C=C.
`-bts` *number*	Torsional sampling level to use in `bmin`. Overrides the `-btc` option and sets it to 1. 0 Restricted 1 Intermediate 2 Enhanced 3 Extended For a definition of the levels, see page 80 of the *MacroModel User Manual*

Table 2. Meta-options for the `ligprep` *command. Suffix values are given for each meta-option that requires a suffix.*

Option	Description
`-adjust_`*suffix*	Adjust to a suitable state. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.
`-expand_`*suffix*	Aggressively expand states. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.
`-retain_`*suffix*	Retain the original state in the output. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*. Suffix values determine which state is kept. If *suffix* is `i`, both the original ionization state and the original tautomer are retained.
`-qik`	Set defaults appropriate for QikProp. Turns on the `desalter` and the `tautomerizer`.
`-unt`	Run `premin` and `bmin` to untangle structures. Used by CombiGlide.
`-vary_`*suffix*	Generate a small number of states. Any combination of `c` (chirality), `i` (ionization states) or `t` (tautomers) can be used for *suffix*.

Table 3. Action performed by meta-options.

Suffix	**Action of** `adjust`	**Action of** `vary`	**Action of** `expand`
`c`	Produce only one stereoisomer	Produce at most 2 stereoisomers	Produce at most 32 stereoisomers
`i`	Produce the ionization state with the lowest overall penalty	Set pH tolerance to 1.0	Set pH tolerance to 2.0
`t`	Produce only the most probable tautomer	Produce at most the 2 most probable tautomers	Produce at most the 8 most probable tautomers

Table 4. Other job options supported by the `ligprep` *command.*

Option	Description
`-HOSTFILE` *filename*	The name of the hosts file to use for this run. The default hosts file is the installed version of `schrodinger.hosts`.
`-INTERVAL` *sec*	The maximum time in seconds between updates of the *jobname*`.log` file.
`-LOCAL`	Do not use a temporary directory for intermediate files. Keep files in the current working directory.
`-WAIT`	Do not return control to the shell until the job finishes.

Table 5. Options for the `para_ligprep` *command, including job control options.*

Option	Description
`-first` *firstlig*	First ligand to include. Default 1.
`-HELP | -h[elp]`	Print usage message and exit.
`-HOSTFILE` *filename*	The name of the hosts file to use for this run.
`-INTERVAL` *sec*	The maximum time in seconds between updates of the *jobname*`.log` file.
`-j` *jobnum*	Subjob number to prepare. Default 0, meaning all subjobs. Must not be negative.
`-JOBCTS` *maxctsjob*	Ensure that each subjob has no more than this many structures to process. Default: 10000.
`-last` *lastlig*	Last ligand to include. Default 0, meaning the last ligand in the file.
`-LOCAL`	Do not use a temporary directory to store the files. Store files in the local directory.

Table 5. Options for the `para_ligprep` *command, including job control options. (Continued)*

Option	Description
`-nproc` *njobs* | `-NJOBS` *njobs*	Divide the overall job into *njobs* subjobs.
`-nx`	Create input files for subjobs and exit; do not run the job.
`-OUTPUT_ORG BY_SUBJOB`	Produce one output file for each subjob.
`-v[er[sion]]`	Report the version number for `para_ligprep`
`-WAIT`	Do not return control to the shell until the job finishes.